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Physica A 336 (2004) 163–173

PHYSICA A

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Diffusion on complex networks: a way to probe their large-scale topological structures

Ingve Simonsen^{a,b,*}, Kasper Astrup Eriksen^{b,c}, Sergei Maslov^d,
Kim Sneppen^{b,e}

^a*Department of Physics, NTNU, NO-7491 Trondheim, Norway*

^b*NORDITA, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark*

^c*Department of Theoretical Physics, Lund University, Sölvegatan 14A, SE-223 62 Lund, Sweden*

^d*Department of Physics, Brookhaven National Laboratory, Upton, NY 11973, USA*

^e*The Niels Bohr Institute, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark*

Received 3 November 2003; received in revised form 12 December 2003

Abstract

A diffusion process on complex networks is introduced in order to uncover their large-scale topological structures. This is achieved by focusing on the slowest decaying diffusive modes of the network. The proposed procedure is applied to real-world networks like a friendship network of known modular structure, and an Internet routing network. For the friendship network, its known structure is well reproduced. In case of the Internet, where the structure is far less well known, one indeed finds a modular structure, and modules can roughly be associated with individual countries. Quantitatively, the modular structure of the Internet manifests itself in an approximately 10 times larger participation ratio of its slowest decaying modes as compared to the null model—a random scale-free network. The extreme edges of the Internet are found to correspond to Russian and US military sites.

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PACS: 89.75.-k; 89.20.Hh; 89.75.Hc; 05.40.Fb

Keywords: Complex random networks; Network modules; Statistical physics

* Corresponding author. Department of Physics, NTNU, NO-7491 Trondheim, Norway. Fax: +47-73597710.

E-mail address: ingves@phys.ntnu.no (I. Simonsen).

1. Introduction

Complex networks are natural structures for representing many real-world systems. Their flexible and adaptive features make them ideal for interrelating various types of information and to update them as time goes by. Recently, there has been tremendous interest, from various fields of science, in the study of the statistical properties of such networks [1,2]. By now, many interesting features of complex networks have been established. So far, the main attention in the study of complex networks has been on the properties of individual nodes and how they connect (link) to their nearest neighbors. However, exploring the *local* properties of the network outside the nearest-neighbor level has not been well studied. A noteworthy exception is the recent study by Girvan and Newman [3]. Such studies will naturally have to address the cluster (modular) structure of the network. To know if a network is modular or not, is important if one tries to assess its robustness and stability, since only a few critical links are responsible for the inter-modular communication in clustered networks. Hence to make the network more robust, such critical links have to be identified and strengthened.

In this work we will address the large-scale topological structures of networks. This problem will be approached by considering an auxiliary diffusion process on the underlying complex network. As it will turn out, it is the slowest decaying diffusive eigenmodes that will be of most interest to us, since such modes will contain, as we will see, information about the weakly interacting modules of the network. Hence, by studying how an ensemble of random walkers slowly reaches a state of equilibrium, one can learn something about the topology of the network.

To study spectral properties of networks is not new; its variants have previously been applied to random graphs [4], to social networks (the correspondence analysis) [5], random and small-world networks (the Laplace equation analysis) [6], artificial scale-free networks [7,8], and community structures [3,9]. A diffusion approach has also made it to practical applications. For instance, the analysis of a diffusion process lies at the heart of the popular search engine Google [10].

2. A Markovian diffusion process on complex networks

The original physical motivation behind the method to be outlined below, was that the relaxation of some arbitrary initial state (of walkers on the network) toward the steady-state distribution, was expected to be *fast* in regions that are highly connected, while *slow* in regions that had low connectivity. By definition, a module is highly connected internally, but has only a small number of links to nodes outside the module. Hence, it was reasoned, that by identifying the slowly decaying eigenmodes of the diffusive network process, one should be able to obtain information about the large-scale topological structures, like modules, of the underlying complex network. We will now formalize this idea and outline the method in some detail.

Let us start by assuming that we are dealing with a (fully connected) complex network consisting of N nodes and characterized by some degree distribution $p(k)$ where k_i denotes the connectivity of node i . Imagine now placing a large number ($\gg N$)

of random walkers onto this network. The fraction of walkers on node i (relative the total number) at time t we will denote by $\rho_i(t)$. In each time step, the walkers are allowed to move randomly between nodes that are directly linked to each other. Since there is no way that a walker can vanish from the network, the total number of walkers must be conserved globally, i.e., one must have $\sum_i \rho_i(t) = 1$ at all times. Furthermore, locally a continuity equation must be satisfied; If we consider, say node i , that directly links to other nodes j , one must require that (the balance equation)

$$\rho_i(t+1) - \rho_i(t) = \sum_j A_{ij} \frac{\rho_j(t)}{k_j} - \sum_j A_{ji} \frac{\rho_i(t)}{k_i} . \quad (1)$$

In writing this equation, we have introduced the so-called adjacency matrix $A_{ij} = A_{ji}$ defined to be 1 if nodes i and j are directly linked to each other, and 0 otherwise [1,2], and k_i , we recall, is the degree of node i , i.e., its number of nearest neighbors $k_i = \sum_j A_{ij}$. The first term on the right-hand side of Eq. (1) describes the flow of walkers into node i , while the last term is associated with the out-flow of walkers from the same node. As will be useful later, Eq. (1) can be casted into the following equivalent matrix form:

$$\partial_t \boldsymbol{\rho}(t) = \mathbf{D} \boldsymbol{\rho}(t) , \quad (2)$$

where $\partial_t \boldsymbol{\rho}(t) = \boldsymbol{\rho}(t+1) - \boldsymbol{\rho}(t)$, and \mathbf{D} is the *diffusion matrix* to be defined below. Eq. (2) should be compared to the continuous diffusion equation for the particle density: $\partial_t \rho(\mathbf{r}, t) = D \nabla^2 \rho(\mathbf{r}, t)$, where D is the diffusion constant. A complex network obviously has an inherent discreteness, and hence no continuous limit can be taken. However, if the continuous diffusion equation is understood in its discrete form, one is lead to regard Eq. (2) as the *master equation* for the random-walk process taking place on the underlying network. By comparing Eqs. (1) and (2), as well as taking advantage of $\sum_j A_{ji} \rho_i(t)/k_i = \rho_i(t)$ (because $\sum_i A_{ij} = k_j$), one is lead to $D_{ij} = A_{ij}/k_j - \delta_{ij}$. Hence, an equivalent formulation of Eq. (2), is

$$\boldsymbol{\rho}(t+1) = \mathbf{T} \boldsymbol{\rho}(t) , \quad (3)$$

where \mathbf{T} is the *transfer matrix* related to the diffusion matrix by $\mathbf{T} = \mathbf{D} + \mathbf{1}$. In component form one thus has $T_{ij} = A_{ij}/k_j$. Since the transfer matrix, “transfers” the walker distribution one time step ahead, it can therefore be thought of as a time-propagator for the process. Formally the time development, from some arbitrarily chosen initial state $\boldsymbol{\rho}(0)$, can be obtained by iteration on Eq. (3) with the result $\boldsymbol{\rho}(t) = \mathbf{T}^t \boldsymbol{\rho}(0)$. Here \mathbf{T}^t means the transition matrix to the t th power.

In general, the transfer matrix (or equivalently, the diffusion matrix) will not be symmetric. However, \mathbf{T} can be related to a symmetric matrix \mathbf{S} by the following similarity transformation $\mathbf{S} = \mathbf{K} \mathbf{T} \mathbf{K}^{-1}$ with $K_{ij} = \delta_{ij}/\sqrt{k_i}$. Thus, \mathbf{T} and \mathbf{S} will have the same eigenvalue spectrum, and all eigenvalues $\lambda^{(z)}$ (of \mathbf{T}) will be real. It is this eigenvalue spectrum that will control the time development of the diffusive process through Λ^t with $\Lambda_{ij} = \delta_{ij} \lambda^{(z)}$. It should be noted that since the total number of walkers is conserved at all times, one must have $-1 < \lambda^{(z)} \leq 1$, and that at least one eigenvalue

should be one.¹ We will here adopt the convention and sort the eigenvalues so that $\alpha=1$ corresponds to the largest eigenvalue $\lambda^{(1)}=1$, $\lambda^{(2)}$ to the next to largest one, and so on. Physically the principal eigenvalue $\lambda^{(1)}=1$ corresponds to a *stationary state* where $\rho(\infty) \propto \rho^{(1)}$, and where the diffusive current flowing from node i to node j is exactly balanced by that flowing from j to i . The stationary state is unique for single component networks, and is fully determined by the connectivities of the network according to $\rho_i(\infty) = k_i / (\sum_i k_i) \propto k_i$. This can be easily checked by substituting this relation into Eq. (3). All modes corresponding to eigenvalues $|\lambda^{(\alpha)}| \neq 1$, are decaying modes since the time dependence of $\rho(t)$ enters through Λ^t and one recalls that $|\lambda^{(\alpha)}| \leq 1$. Notice that $\lambda^{(\alpha)} > 0$ represent non-oscillatory modes, while $\lambda^{(\alpha)} < 0$ correspond to states where oscillations will take place with time, but this latter possibility will not be considered here.

The large-scale topology of a given complex network reflects itself in the statistical properties of its diffusion eigenvectors $\rho^{(\alpha)}$. One such property is the participation ratio (PR), that will be defined below. It quantifies the effective number of nodes participating in a given eigenvector with a significant weight. Since the stationary state of a network depends on the connectivities of its nodes, $\rho_i(\infty) \propto k_i$, it is convenient to introduce a normalized eigenvector

$$c_i^{(\alpha)}(t) = \frac{\rho_i^{(\alpha)}(t)}{k_i}. \quad (4)$$

Observe that $c_i^{(\alpha)}$ is nothing but the walker density per link of node i . Hence, in effect, $c_i^{(\alpha)}$ represents the *outgoing currents* flowing from node i , along each of its links, toward its neighbors. In the steady state, where $\rho_i(\infty) \propto k_i$, it follows that these currents are all the same for any link in the network. Hence, highly connected nodes are not treated differently from less connected nodes. More formally, $\mathbf{c}^{(\alpha)}$ are the eigenvectors of the transposed transfer matrix \mathbf{T}^\dagger corresponding to the same eigenvalue $\lambda^{(\alpha)}$ (of \mathbf{T}). Here one alternatively could have defined \mathbf{T}^\dagger (instead of \mathbf{T}) as the transfer matrix from the very beginning. Doing so, would have resulted in a master equation of the form (3), but for the currents $\mathbf{c}(t)$ with corresponding eigenmodes $\mathbf{c}^{(\alpha)}$. The physical interpretation of such an alternative equation is as follows: Instead of walkers, think of a signal propagating on the underlying network. The signal at node i at time $t+1$ is then the average of the signal at the nearest neighbors at time t .

If the link currents are normalized to unity, i.e., if $\|\mathbf{c}^{(\alpha)}\|_2 = 1$ in the L_2 -norm, then the PR is defined as [11]

$$\chi_\alpha = \left[\sum_{i=1}^N \left(c_i^{(\alpha)} \right)^4 \right]^{-1}. \quad (5)$$

For the stationary state, where all the currents are equal to $c_i^{(1)} = 1/\sqrt{N}$, one has $\chi_1 = N$, where we recall that N is the total number of nodes in the network. Hence, when $\alpha \neq 1$, the ratio χ_α can be regarded as an effective number of nodes participating

¹ For the diffusion matrix, this means that its spectrum, $\{\lambda_D^{(\alpha)}\}$, must satisfy $-2 < \lambda_D^{(\alpha)} \leq 0$ since $\lambda_D^{(\alpha)} = \lambda^{(\alpha)} - 1$.

in the eigenvector $\mathbf{e}^{(\alpha)}$ with a significant weight [11,12]. It should be noted that the participation ratio is a simple and crude measure of size. Strictly speaking, for this ratio to be able to say something with confidence about the size of a given module, the main contribution to χ_α should come from nodes within that module. For instance, if χ_α gets major contributions from current elements $c_i^{(\alpha)}$ of different signs, i.e., from different topological structures, it is not trivial to relate χ_α to the size of a single module.

For all types of complex networks where a modular structure is of interest, it is important to try to quantify the number of modules. Such information is of interest since this number may say something about the organizing principles being active in the generating process of the network. However, the measurement of this number is often hampered by statistical uncertainties due to temporary (non-robust) topological structures being counted as modules. Hence the challenge is to obtain the significant (or robust) number of modules that are due to the “rule of creation” and not just happened to be there by chance. For this purpose, it is useful to introduce a null model—a randomized version of the network at hand—but so that the degree distribution of the original network is not changes [13]. A rough estimate of the number of different modules contained in a network could be given by the number of slowly decaying non-oscillatory modes that have a participation ratio, χ_α , significantly exceeding the (ensemble) averaged participation ration of the corresponding randomized network, χ_α^{RD} . Hence, it is suggested that a module is significant if $\chi_\alpha \gg \chi_\alpha^{\text{RD}}$.

We will close this section by noting that the (outgoing) currents, c_i^α , can also be used for vitalization purposes. The basis of this approach is the observation that the outgoing currents on links within a module are almost constant, and the size of this constant depends on to which extent the module participates in the given eigenmode. The constants thus varies from module to module and from eigenmode to eigenmode. Hence, by sorting $c_i^{(\alpha)}$ by size, nodes belonging to the same module will be located close to each.

3. The datasets

During a 2 year period in the mid 1970s, Zachary studies the relations among 34 members of a university karate club during a period of trouble [14]. A serious controversy existed between the trainer of the club (node 1 in Fig. 1a) and its administrator (node 34). Ultimately, this conflict resulted in the breakup of the club into two new clubs of roughly the same size. In his original study [14], Zachary mapped out the strength of friendship between the various members. In our study, however, we will be considering the unweighted version of his network [15] (see Fig. 1a). Recently, this same network was used by Girvan and Newman [3] in their study of community structures.

The second network that will be considered is a much larger network taken from the organization of the Internet. The Internet consists of a large number of individual computers that are identified by their so-called IP-address, and they are usually grouped together in local area networks (LAN). Such computer networks are connected to one another via routers—a complex network linking device. In addition to being able to

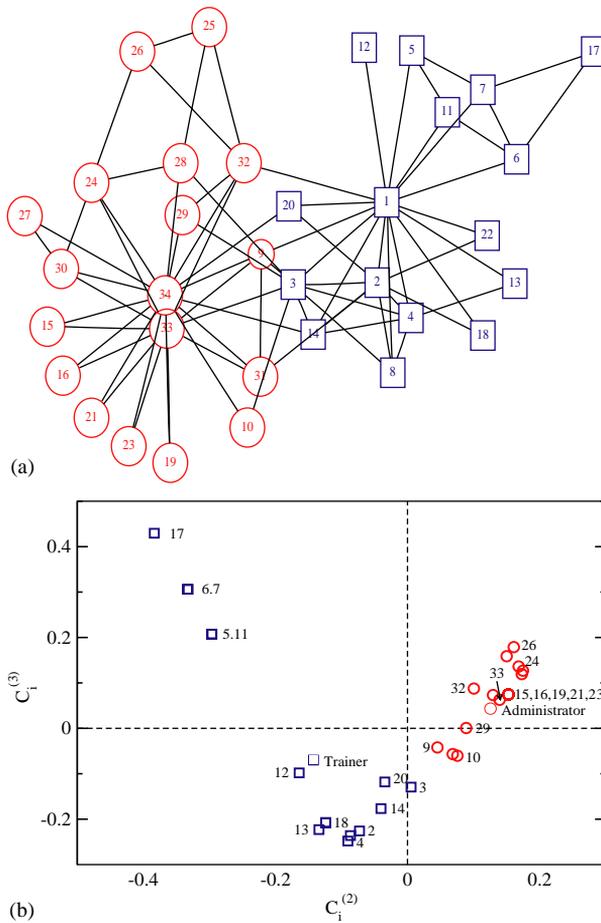


Fig. 1. Top panel (a): Zachary’s friendship network [14] of the “troubled” karate club consisting of $N = 34$ nodes and $L = 78$ links (figure after Ref. [3]). Here open squares and circles are used to denote the supporters, in the ongoing conflict, of the trainer (node 1) and administrator (node 34), respectively. Bottom panel (b): The $C^{(2)}C^{(3)}$ -plot maps out the large scale topology of the network. The dashed lines indicate the lines of zero currents.

direct pieces of information to its intended destination, a router also has the ability to determine the best path to a given destination (routing). This is done by keeping available an updated routing table telling the router how to reach certain destinations specified by the network administrator. In much the same way as computers are being organized into networks, the same is done for routers. If the router network becomes large and coherent enough, it may make out what is called an *autonomous system* (AS). An AS is a connected segment of a network that consists of a collection of subnetworks (with hosts attached) interconnected by a set of routes. Usually, it is required that the subnetworks and the routers should be controlled by a coherent organization—like, say, a university, or a medium-to-big enterprise. Importantly for the efficiency of the

Internet, each AS, identified by a unique AS number, is expected to present to the other systems a consistent list of destinations reachable through that AS, as well as a coherent interior routing plan.

The particular network we will be considering is an AS network collected by the Oregon Views project on January 3, 2000 [16]. In this network the AS will act as nodes, while their routing plans, i.e., with which other AS a given one directly shares information, will correspond to the links of the network.

4. Results and discussion

4.1. The Zachary friendship network

In Section 2, it was argued that from the currents corresponding to the *slowly* decaying eigenmodes, one should be able to map out the large-scale structure of the underlying network. Our hypothesis will now be put to the test, and we start with the small friendship network due to Zachary [14]. This network is depicted in Fig. 1a, and it is small enough to enable us to see how it all comes about. By visual inspection of this figure, it is apparent that there are, at least, two large-scale clusters—one corresponding to the trainer of the karate club (node 1) and his supporters, and one to the administrator (node 34). In Fig. 1a, the karate club members (according to Zachary) supporting the trainer in the ongoing conflict are marked with squares (16 nodes), while the followers of the administrator are marked with open circles (18 nodes). Notice that this subdivision was done by Zachary [14], and no sophisticated clustering techniques were applied to obtain these results.

We will now see if the same clustering structure can be obtained by the method outlined in Section 2 of this paper. Let us start by considering the two most slowly decaying modes of the network, namely $\alpha=2$ and 3 (with our ordering), corresponding to the eigenvalues $\lambda^{(2)}=0.87$ and $\lambda^{(3)}=0.71$, respectively. If one sorts the elements of the current vector $\mathbf{c}^{(2)}$ by size, and group them according to their signs, one recovers two clusters (see the abscissa of Fig. 1b). This grouping, or topological structure, fits nicely with the original assignments made by Zachary (Fig. 1a) and indicated by the open squares and circles in Fig. 1b. Hence it is the trainer–administrator separation of the karate club members that is mapped out by the $\mathbf{c}^{(2)}$ -currents. Observe that node 3, which has an equal number of links to supporters of the trainer and administrator, has a current that is almost zero. Our identification of this node is the only one that differs from that made originally by Zachary. Interestingly, our classification, including node 3, fits that previously obtained by Girvan and Newman [3] in their hierarchical tree clustering approach.

If the same procedure was repeated, but for the currents $\mathbf{c}^{(3)}$, one would map out other topological features of the network. In Fig. 1b, a $c^{(2)}c^{(3)}$ -plot is presented. Such a plot groups the nodes along two axis; the $c^{(2)}$ -axis—corresponding to the trainer–administrator axis—and the $c^{(3)}$ -axis. The most striking feature of Fig. 1b is the group of nodes corresponding to $c^{(2)} < 0$ and $c^{(3)} > 0$, i.e., to the following group of nodes {5–7, 11, 17}. In Fig. 1a, these nodes are located in the upper left corner of the graph.

They are in addition to being connected among themselves, only connected to the rest of the network via the trainer. Thus, they represent a sub-cluster, and this is indeed what is apparent from Fig. 1b.

The participation ratios for the two slowest decaying diffusive modes were found to be $\chi_2=14.0$ and $\chi_3=13.1$, respectively. As can be seen from Fig. 1b, these participation ratios receive substantial contributions from both positive and negative current elements, i.e., from more than one topological structure. Hence, we suspect that these numbers being close to the size of the administrator and trainer “clan” (of size 18 and 16 nodes, respectively) is somewhat accidental.

4.2. The autonomous system network

We will now focus our attention on the AS network introduced in the previous section. This network, consisting of $N = 6474$ nodes and 12,572 undirected links, is so big that plotting it for the purpose of study its modular structure is not a practical option. Motivated by what we found for the small Zachary friendship network, we will now go ahead and use somewhat similar techniques for its study.

In Fig. 2 the participation ratio, χ_α , of eigenvectors $c_i^{(\alpha)}$ (top) and the eigenvalue density (bottom) are plotted as functions of the corresponding eigenvalues $-1 < \lambda^{(\alpha)} < 1$. The data for the Internet, that is an example of a scale-free network [17], are displayed together with the data for its randomized counterpart (the null model). From Fig. 2 it is apparent that while the density of states is rather similar for these two networks, the participation ratios of the slowly decaying modes, especially for $\lambda^{(\alpha)}$ close to 1, are markedly higher in the Internet network than in the accompanying randomized network. These differences signal large-scale topological structures [12] that are real and not accidental. For the most slowly decaying diffusive eigenmode, the participation

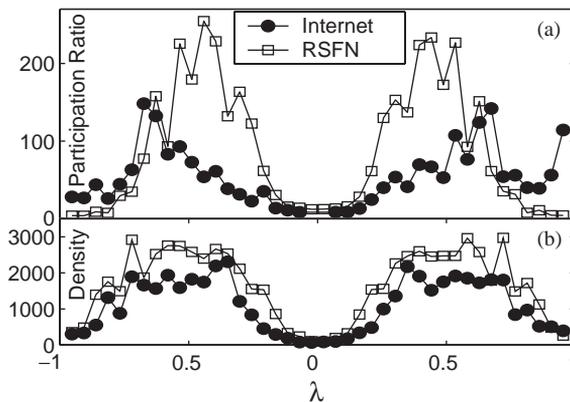


Fig. 2. The participation ratio χ_α (top, a) and the eigenvalue density (bottom, b) as a function of the eigenvalue of the transfer matrix, $-1 < \lambda^{(\alpha)} < 1$, measured in the Internet (filled circles) and in its randomized counterpart (open squares)—a random scale-free network. The participation ratio was averaged over λ -bins of size 0.05 excluding eigenmodes $\lambda^{(\alpha)} = 0$, and $\lambda^{(1)} = 1$ (cf. Ref. [12]).

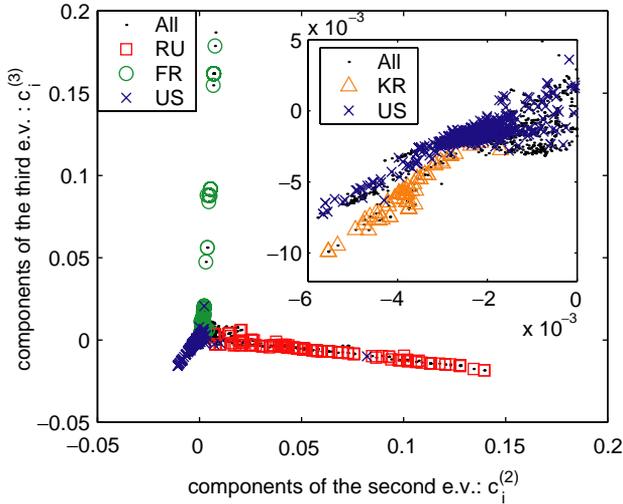


Fig. 3. The Internet clustering: The coordinates of the i th AS in this plot are its current components $(c_i^{(2)}, c_i^{(3)})$ of the two slowest decaying non-oscillatory diffusion modes. The symbols reveals the geographical location of the AS: Russia—squares, France—circles, USA—crosses, Korea—triangles). Note the straight lines corresponding to good country-modules.

ratio is $\chi_2 \simeq 100$ (cf. Fig. 2a). From Fig. 3, that depicts the currents of the two slowest decaying diffusive eigenmodes, one observes that the main contribution to χ_2 comes from current elements $c_i^{(2)}$ of the same sign. Thus, a module has been detected, and χ_2 roughly measures its size. From, Fig. 3 one also makes the interesting observation that the main contributing nodes to χ_2 are AS located in Russia (denoted by open squares in Fig. 3). Hence, the diffusive mode $\alpha = 2$ maps out Russia, as a Russian module [12]! In total there are 174 Russian nodes in our dataset. Moreover, from Fig. 3, modules corresponding to countries like the USA, France and Korea are also easily identified. The edges of the AS Internet network, defined as the nodes corresponding to the most distant values of the current elements $c_i^{(2)}$, are in this case represented by a Russian and a US military site located in the South Pacific. These nodes can thus be said to represent the extreme edges of the Internet. One has also studies the number of significant modules (where $\chi_\alpha \gg \chi_\alpha^{\text{RD}}$), and found that this number for the AS network is roughly $M = 100$ [12]. The number of different nodes participating in one or more of these M modules was found to be about $N_M \sim 1800$. Hence the modularity of the network is (at least) $N_M/N \simeq 30\%$.

4.3. Generic features of the current–current plots

One common feature of the current–current plots, Figs. 1b and 3, is their line or star-like structures. Such structures are in fact rather generic, and we will here try to explain why. We have argued earlier that current elements $c_i^{(a)}$ should almost be the same within a module. Hence, for two nodes i and j belonging to one and the same

module, the fraction $c_i^{(\alpha)}/c_j^{(\alpha)}$ is expected to be a constant unique for that module, but independent of the diffusive mode α . For two different (significant) diffusive modes, say α and β , the fraction $\gamma = c_i^{(\alpha)}/c_i^{(\beta)}$ (for node i) will therefore as a consequence also be constant. Thus, under the assumptions made above, one predicts a straight line in a current–current plot (that passes through the origin) [12]: $c_i^{(\alpha)} = \gamma c_i^{(\beta)}$, for nodes i belonging to the same module. From Fig. 3, this simple argument appears to be valid. That Fig. 1b seems to not pass through the origin, but still being straight lines, we believe is due to the diffusive modes being excited over a non-trivial background in this case.

4.4. Numerical implementation

Before presenting the conclusions of this paper, we will add a few closing remarks on the numerical implementation of the method. For this work to have any relevance for large real-world networks, a fast, memory saving, and optimized algorithm for the calculation of the largest eigenvalues and the corresponding eigenvectors of a sparse matrix is required. Fortunately, such an algorithm has already been implemented and made available e.g. through the TRLan software package [18]. This software is optimized for handling large problems, and it can run on large-scale parallel supercomputers.

5. Conclusions

We have generalized the normal diffusion process to diffusion on (discrete) complex networks. By considering such a process, it has been demonstrated that topological properties—like modular structures and edges—of the underlying network can be probed. This is achieved by focusing on the slowest decaying eigenmodes of the network. The use of the procedure was exemplified by considering a small friendship network, with known modular structure, as well as a routing network of the Internet, where the structure was not so well known. For the friendship network the known structure was well reproduced, and the Internet was indeed found to be modular. The detected modules of the Internet were consistent with the geographical location of the nodes, and the individual modules corresponded roughly to the national structure. Interestingly, it was observed that a political subdivision of the Internet was also one of the predictions of the algorithm presented in this paper; The two most poorly connected nodes of the Internet (extreme edges), were found to be represented by a Russian and a US military site located in the South Pacific.

Acknowledgements

Work at Brookhaven National Laboratory was carried out under Contract No. DE-AC02-98CH10886, Division of Material Science, US Department of Energy.

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